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Numerical Simulations of Experimental Fireball and Blast Wave from a High-Pressure Tank Rupture in a Fire

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ABSTRACT

Hazards from the fireball and blast wave after high-pressure hydrogen tank rupture in a fire are not yet fully understood. The contemporary tools like CFD are not yet validated against experimental data to be used as a reliable predictive tool for such catastrophic failures. In this study the experiment with high-pressure hydrogen storage tank rupture in a fire, followed by a blast wave and a fireball, was numerically simulated. The applied CFD model includes the eddy dissipation concept (EDC) sub-model for combustion incorporating a detailed chemistry with 37 chemical reactions, and the RNG k-epsilon sub-model for turbulence. The model has been recently successfully applied to simulate experimental data on spontaneous ignition of hydrogen during the sudden release into the air, and different indoor jet fire regimes. In this study, the results of the simulations are compared against experimental data on a high-pressure (35 MPa) stand-alone hydrogen tank of volume 72.4 l rupture in a bonfire test. The simulation results are compared with predictions of the analytical model too. The CFD model gives insights into the dynamics of the blast wave and the fireball to assess the hazard distances. The simulations reproduced well experimental parameters such as blast wave decay, overpressure dynamics at different distances, including the timing of the blast wave arrival, fireball shape and size.

KEYWORDS: Analytical model, blast wave, CFD, experiment, fireball, fire, tank rupture.

INTRODUCTION

The use of hydrogen under high pressure could pose serious problems in the case of fire, if thermally activated pressure relief device (TPRD) failed to be activated and the storage tank is not thermally protected. The use of contemporary tools like computational fluid dynamics (CFD) helps to gain insights into the phenomena to tackle the issue. Combustion in the fireball can be characterised as partially premixed. Both phenomena, i.e. blast wave and fireball, have to be understood and predictive engineering tools to be developed for assessment of safety distances for hydrogen systems and infrastructure.

The first attempt to simulate phenomena of blast wave and fireball from the tank rupture in a fire have been undertaken by the authors recently [1]. The realizable k - ϵ turbulence model [2] along with the Eddy Dissipation combustion model [3] with infinite rate chemistry were applied. It was demonstrated that this CFD model underestimates the experimental data for both the fireball size and the blast wave decay. Due to its nature the model did not allow the detailed analysis of combustion inside the fireball. Therefore, the Eddy Dissipation Concept (EDC) model with finite chemistry is applied in this study.

The harm to people and damage to buildings after the high-pressure flammable gas tank rupture in a fire can be done by pressure and impulse effects of the blast wave, and thermal effects of the fireball temperature and radiation. Paper [4] describes the novel dimensionless correlation for hydrogen jet fires and the methodology to calculate hazard distances. Three different hazard distances for jet fire were defined following three harm criteria for people from hot gases [5]: “no

harm” limit (70°C), “pain” limit (115°C for 5 min exposure) and “fatality” limit (third degree burns at 309°C for 20 s exposure). The study [6] presents a novel model of the blast wave decay after high-pressure tank with flammable gas ruptures in a fire, which accounts for the first time the contribution of combustion into the blast wave strength contrary to existing models. The model reproduced available experimental data and recommended as a predictive engineering tool for calculation of hazard distances due to a blast wave. Three harm to people criteria were considered by the authors [6] to assess hazard distances: “no harm” distance where pressure is less than 1.35 kPa, “injury” distance at overpressure of 16.5 kPa (direct effect of pressure wave with 1% injury), and “fatality” distance at overpressure of 100 kPa. The same criteria are applied in this study for the assessment of hazard distances from the blast wave and the fireball.

The aim of this study is modelling and simulation of the blast wave and the fireball dynamics observed in the experiment and validation of the CFD model for use as a contemporary tool for hydrogen safety engineering.

BONFIRE TEST EXPERIMENTAL SETUP AND RESULTS

The only experimental data available in the open literature up to date on hydrogen tank rupture in the bonfire test without TPRD are described in [7]–[10]. The stand-alone Type 4 tank bonfire test [7], [8] was selected for the model validation in this study. The external size of the tank was 0.84 m in length, 0.41 m in diameter, with internal volume of 72.4 l. The storage pressure was 34.3 MPa at the beginning of the test. The tank was placed 0.2 m above the ground over a propane burner with heat release rate of 370 kW as shown in Fig. 1 (left). The tank ruptured in the fire after 6 min 27 sec of exposure. The pressure sensor locations are shown in Fig. 1 (right). The measurements demonstrated the blast pressures 300 kPa, 83 kPa and 41 kPa at 1.9 m, 4.2 m and 6.5 m respectively, and the maximum diameter of the fireball about was 7.7 m.

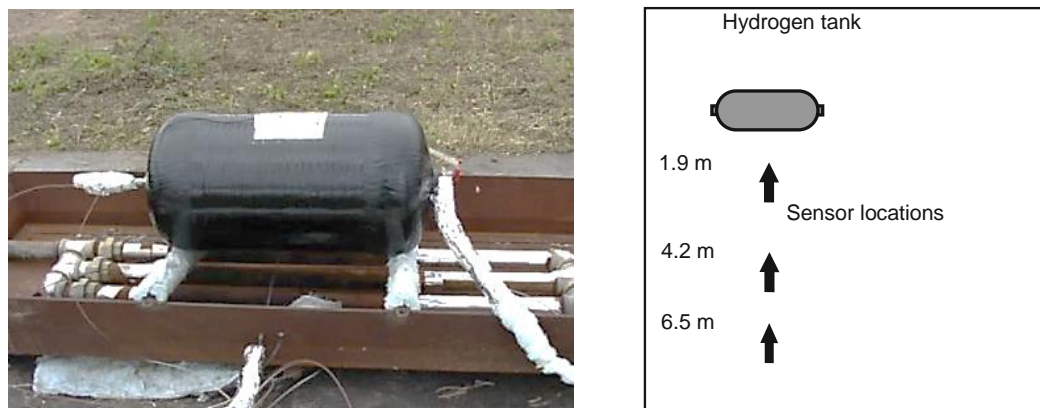


Figure 1. Test setup (left) and pressure sensor locations (right) [8].

CFD MODEL, GEOMETRY AND GRID

The renormalization group (RNG) k - ε turbulence model is applied in this study similar to our previous simulations of hydrogen jet fire indoors [11]. The RNG model by Yakhot and Orszag was derived from the instantaneous Navier-Stokes equations and described in [12], [13]. The analytical derivation resulted in a model with constants different from those in the standard k - ε model, and additional terms and functions in the transport equations for k and ε . The compressible solver with ideal gas model (pressure in a starting shock is below 10 MPa for

hydrogen storage applications) for calculation of density was applied in contrast to incompressible solver used in our previous study of indoor fires with EDC model [11].

The EDC model applied for simulation of combustion is an extension of the eddy dissipation model with inclusion of chemical reaction mechanism in a turbulent flow [14]. The chemical reaction mechanism [15] of hydrogen combustion in air employing 37 elementary reactions and 13 species is applied. This is similar to numerical simulations of spontaneous ignition of hydrogen during sudden release into T-shaped pressure relief device in the study [16], where experimental data were reproduced to confirm the predictive power of the EDC model and the employed simulation approach.

In this study simulations were performed using ANSYS Fluent compressible pressure-based solver with PISO pressure-velocity coupling algorithm, which is recommended for a transient flow calculations, especially when a large time step is applied. The spatial discretization for the gradient was least squares cells based, the second order upwind scheme for convective terms of pressure, density, momentum and species equations, and first order upwind scheme for convective terms of k and ε equations. The transient formulation was the first-order implicit and the gravity forces were applied.

Since the solver with implicit time stepping was used in the simulation the Courant–Friedrichs–Lewy (CFL) number was kept below 1 throughout the whole duration of the simulation by controlling the time step as shown in Table 1. The number of iterations per time step was set to 30.

Table 1. Time step values in simulation.

Simulated time, s	0-0.025	0.025-0.04	0.04-0.065	0.065-0.2	0.2-0.6	0.6-1.0
Time step, s	1e-6	1e-5	2e-5	4e-5	1e-4	2e-4

In order to improve the solution convergence and suppress numerical instabilities, which may occur due to 2nd order discretisation scheme, the high order term relaxation (HOTR) factor of 0.75 was applied for all variables. When spatial discretization higher than 1st order is used it is shown to prevent convergence stalling in some cases. Such high-order terms can be of significant importance in certain cases and lead to numerical instabilities. This is particularly true at aggressive solution settings such as tank rupture by instantaneous disappearance of the wall. In such cases, high order relaxation is a useful strategy to minimize user's interaction during the solution. This can be an effective alternative to starting the solution with the first order, and then switching to the second order spatial discretization at a later stage.

In simulations of the tank rupture high gradients of velocity and pressure occur in the vicinity of the tank walls. Tetrahedral mesh would be not suitable for flow simulations with large velocity gradients [17]. The major disadvantage of tetrahedral mesh is that control volumes have only four neighbours, so computing gradients can be problematic because neighbouring nodes may all lie in nearly one plane. This will result in stiff evaluation of the gradient in the direction normal to the shock wave. To resolve this problem, a polyhedral grid shown in Fig. 2 with the total number of control volumes CV=172,199 was built by the conversion from the tetrahedral grid used in our study [1] and which consisted of significantly larger number of CV=976,294. The polyhedral grid can overcome the aforementioned disadvantage, so the gradients can be much better approximated.

The computational domain has a hemispherical shape of 100 m in diameter as shown in Fig. 2. The size and the shape of the domain are determined by taking into account the blast wave and the fireball radius and to reduce the influence of the domain boundary on the solution. Figure 2

shows that the domain was divided into sub-zones with different degree of resolution, with better refinement close to the tank and the zone of the fireball. The fireball zone was 20 m in diameter, the near tank hemisphere was 2 m in diameter, and the tank itself was 0.66 m in length and 0.37 m in diameter with the total volume of 72.4 l.

The initial conditions for the simulation were set same as in the experiment [8] just at the moment of the tank burst. Hydrogen mass fraction in the tank was set to 1, initial pressure to 35 MPa and its temperature to 312 K. The non-slip impermeable adiabatic boundary condition was applied at the ground. The pressure outlet condition was set as the domain boundary with ambient temperature of 293 K and pressure of 101,325 Pa. The tank rupture was modelled as the instantaneous disappearance of the tank wall.

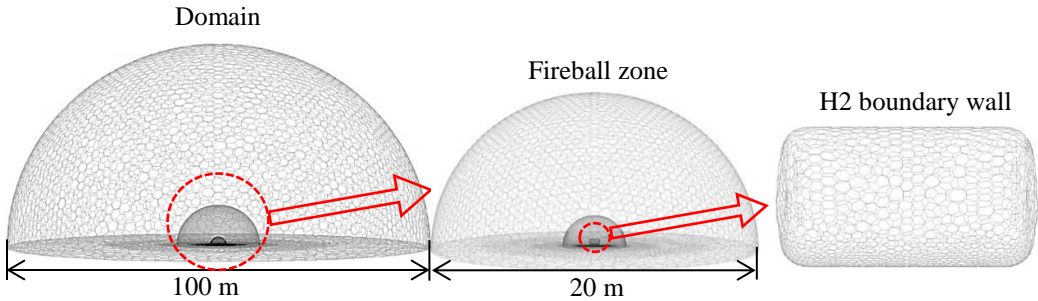


Figure 2. The computational domain and the grid: side view of the domain (left), side view of the fireball zone (centre), and the tank boundary wall grid (right).

RESULTS AND DISCUSSION

Blast wave decay

The simulation starts with the instantaneous removal of the tank wall. This generates the starting shock propagating outwards [6]. Then, the spontaneous ignition of hydrogen in air is observed in simulation at the contact surface between heated by the shock air and expanding hydrogen. This numerical ignition imitates the ignition in the experiment from the surrounding the tank fire. In reality, the spontaneous ignition observed in the simulations is probably not possible due to finite time of tank wall removal. Experimental data and results of blast wave decay prediction by analytical model and numerical simulations are shown in Fig. 3.

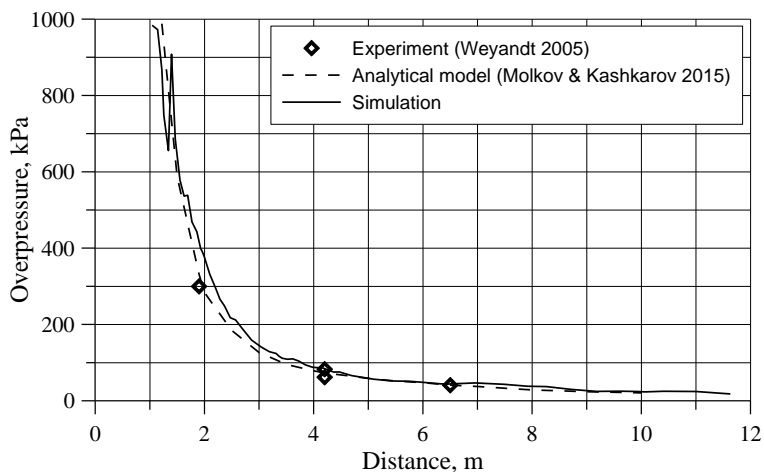


Figure 3. Comparison between experimental, analytical and numerical overpressure versus distances.

The analytical model [6] is the real gas model that accounts for contribution of combustion into the blast wave strength (dashed curve). The analytical model was calibrated against this experiment (diamonds) and, not surprisingly, reproduces it well. The simulated maximum overpressure (solid line) is somewhat above the experiment at distance 1.9 m. However, experimental overpressures are reproduced well at distances 4.2 and 6.5 m from the tank.

Transient blast wave overpressure at different distances

The pressure dynamics at three locations of pressure sensors is shown in Fig. 4. The experimental pressure transients have sharper fronts at 4.2 m and 6.5 m compared to the simulated pressure. This can be explained by the fact that any discontinuity in simulations, including shock wave, requires 3-5 control volumes and that the grid resolution further from the tank is 10 times coarser than in the vicinity (cell size at location of sensor 1.9 m is 4 cm, and at location of sensors 4.2 and 6.5 m is 40 cm). In the experiment, a part of mechanical energy of compressed gas was lost due to ground cratering, etc. In the simulation the ground boundary is reflecting the shock without losses. This could partially explain the over-prediction of pressure nearby the tank at distance 1.9 m. Other possible reasons of the higher pressure peak at sensor location 1.9 m in simulations is higher value of mechanical energy (coefficient 1.8 instead of 2 was used in [6] following accepted practice), and the use of ideal instead of real gas in the simulations that gives a higher value of stored mechanical energy.

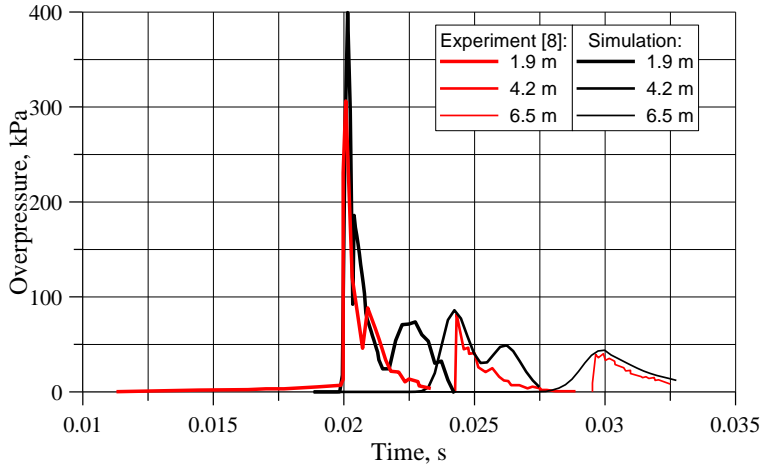


Figure 4. Transient overpressures simulation versus experiment [8].

Fireball size and shape

The maximum diameter of visible fireball in the stand-alone tank test was reported as 7.6 m [9], with the analytical model value of 11.8 m [6]. The analytical model is based on the calculation of diameter of hemisphere, which would be occupied by combustion products of stoichiometric hydrogen–air mixture, assuming that all released hydrogen is consumed. This diameter is the maximum distance until which the release of chemical energy contributing to the blast wave strength is accounted for in the analytical model. The simulations results in Fig. 5 show that 1 s after the tank rupture the fireball diameter determined by hydroxyl (OH) concentration is about 10.5 m, and about 12 m if determined by temperature. These values are closer to the analytical model prediction rather than to the experiment. The simulation reproduced experimental observation that the fireball lifted off the ground by about 1 s (see Fig. 5).

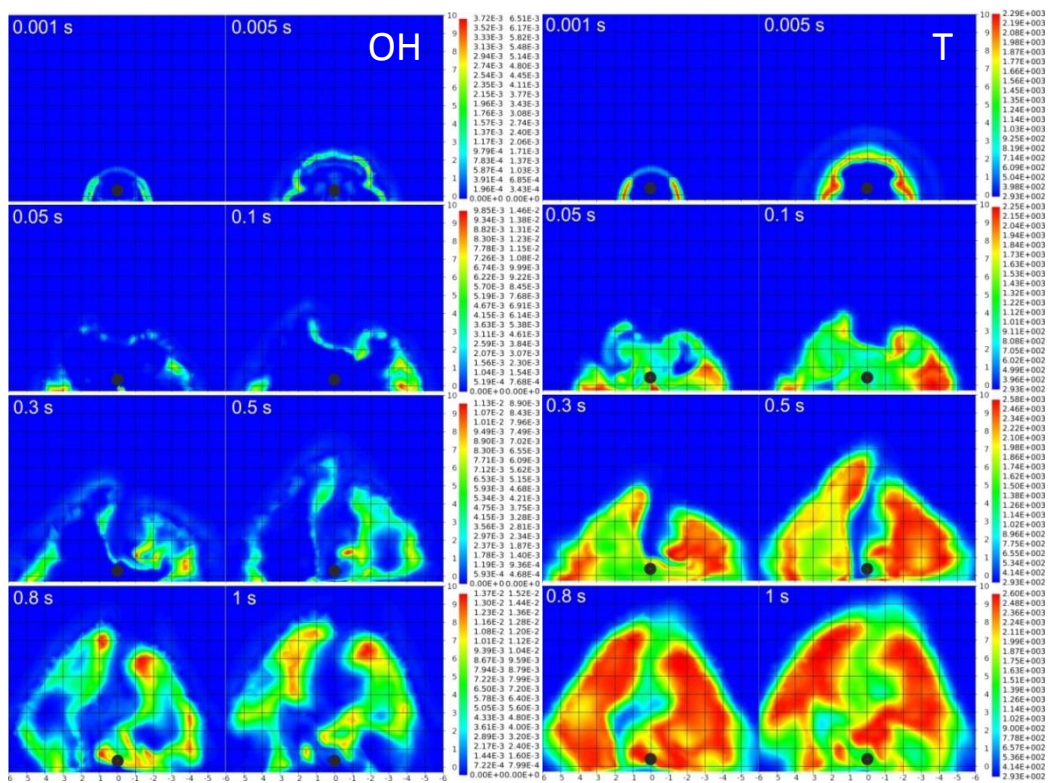


Figure 5. The simulated dynamics of fireball: OH mole fraction in the range (0-0.015) (left), temperature (293-2600 K) (right).

Figure 6 shows the comparison of experimental fireball size of 7.6 m at time 45 ms reported in [7] with centreline snapshots of temperature and hydroxyl in the simulations. It can be seen that the size and the shape of the fireball are very close to the experimentally observed values.

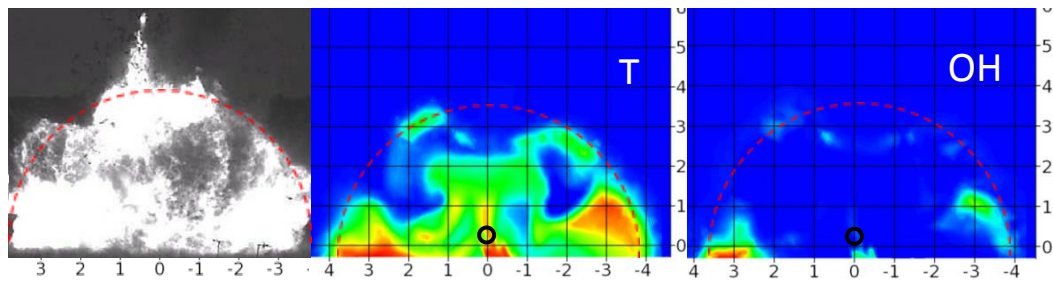


Figure 6. Snapshot of experimental fireball at time 45 ms after the tank rupture (left) versus simulated snapshots of temperature (293-2570 K) (middle), and OH mole fraction in the range (0-0.011) (right).

Hazard distances

Let us compare the CFD model assessment of hazard distances for humans with the analytical model calculations. The hazard distances to people outdoors are determined by the blast wave

pressure threshold as accepted in [6], and by temperature thresholds as described in [5] (see Table 2). The analytical model prediction and the CFD model results are very close to each other. The CFD values are conservative with the overestimation within 8%. Three hazard distances determined by temperature harm criteria are close to each other and are in the range 6-7 m. It is worth mentioning that the harm to people from fireball radiation is out of the scope in this study. It can be concluded from the table that the “fatality” hazard distance determined by the fireball temperature is almost 1.5 times longer than the hazard distance calculated by the blast wave pressure. However, for the “injury/pain” criteria the blast wave hazard distance is twice longer compared to the temperature hazard distance. The “no harm” hazard distance cannot be compared accurately as the calculation domain size of 50 m was insufficient for blast wave decay to “no-harm” pressure limit of 1.35 kPa (the analytical model prediction is 72.5 m). “No-harm” separation distance by the blast wave is 10 times longer than the the separation distance calculated by the fireball temperature.

Table 2. Hazard distances to humans in meters determined for blast wave and temperature harm criteria by the CFD model and the analytical model [4], [6].

Harm criteria for blast wave/temperature	CFD model	Analytical model
No harm: (1.35 kPa)/(70°C)	(3.3 kPa at 50 m) ^a /7	72.5/-
Injury/pain: (16.5 kPa)/(115°C)	12.5/6.5	11.5/-
Fatality: (100 kPa)/(309°C)	3.7/6	3.5/-

^aOverpressure measured at the computational domain boundary 50 m.

The propagation dynamics of the blast wave zone with overpressure above the “injury” threshold of 16.5 kPa is shown in Fig. 7. Shock reflections and rarefaction waves are responsible for pressure oscillations in the tank vicinity as seen in Fig. 3. After 2.2 ms pressure in the tank location is always below the “injury” threshold. Figure 7 shows that the blast wave has a sharp hemispherical shape. This is different from the distribution of the reaction zone visualised by mole fraction of hydroxyl OH and the temperature within the fireball cross-section (see Fig. 5), which is highly non-uniform and distributed throughout the space behind the shock as was previously assumed in the analytical model of the blast wave decay [6].

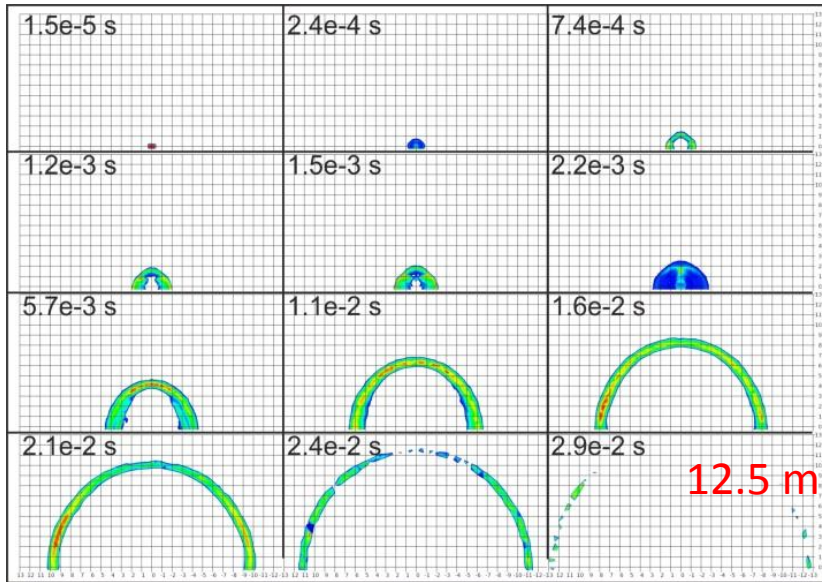


Figure 7. The simulated dynamics of blast wave (separation 16.5 kPa 1% injury threshold).

CONCLUSIONS

The CFD model based on the RNG $k-\varepsilon$ turbulence sub-model and the EDC combustion sub-model was validated against the experimental data on high-pressure hydrogen tank rupture in a fire, including blast wave pressure dynamics at different distances, fireball size and shape, and timing of the fireball and blast wave arrival. The model is capable to reproduce the phenomena of blast wave and a fireball with accuracy sufficient for hydrogen safety engineering. It can be applied as a contemporary tool for hydrogen safety engineering to assess the hazard distances in the case of catastrophic rupture of high-pressure hydrogen storage tank in a fire.

The “no-harm” distance by blast wave is shown to be longer compared to the separation distance by temperature of the fireball. However, the assessment of hazard distance due to radiation from the fireball was out of the scope in this study and yet to be carried out. This is the subject of our ongoing research to be published shortly.

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